Nonequilibrium Alloys in Systems with Positive Heat of Mixing

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Icosahedral Local Order Demonstrated in a Non-Quasi-Crystal Forming Amorphous Alloy

- The atomic arrangements in amorphous matters (liquids and solids) are much less understood than in crystals. Icosahedral local order (ILO) has long been hypothesized to be present. Previous evidence for ILO in amorphous solids are found in systems that form quasi-crystals, where the local clusters with five-fold symmetry may well be embryos of an icosahedral phase.

- We used reverse Monte Carlo (RMC) simulation of the EXAFS as well as x-ray scattering data to construct a structural model for the amorphous Ag-Ni alloy. Upon crystallization, this system forms no quasi-crystals and in fact no ordered structures other than fcc.

- Our direct observation (see figure) based on a common-neighbor analysis indicates that icosahedral and distorted icosahedral short-range order indeed dominate in the amorphous state. This appears to be an intrinsic feature that also explains the barrier to the nucleation of fcc crystals.

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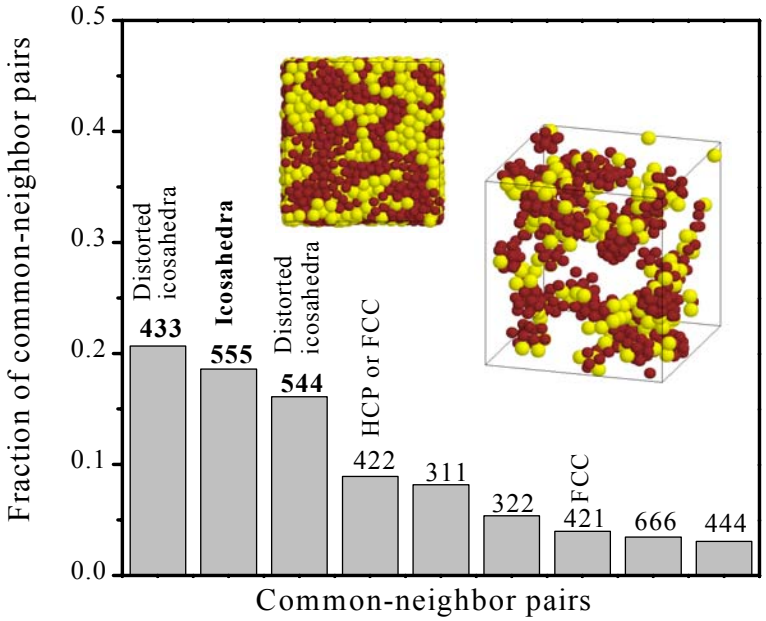
W.K. Luo, H.W. Sheng, F. Alamgir, J.M. Bai, J.H. He and E. Ma, "Icosahedral Short-Range Order in an Amorphous Alloy", *Physical Review Letters*, in revision (2003).



Fractions of various common-neighbor pairs in the $Ni_{60}Ag_{40}$ amorphous alloy. The three dominant ones are all related to ILO. The inset shows the 3D configuration of 48 interpenetrating and interconnected perfect icosahedral clusters. The red spheres are Ni atoms, and the yellow balls are Ag.